PNNL Perspective on Grand Challenges in Materials Research in Support of GNEP

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Materials Under Irradiation
(Microstructure Evolution and Characterization)

Multiscale Methods

ab-initio
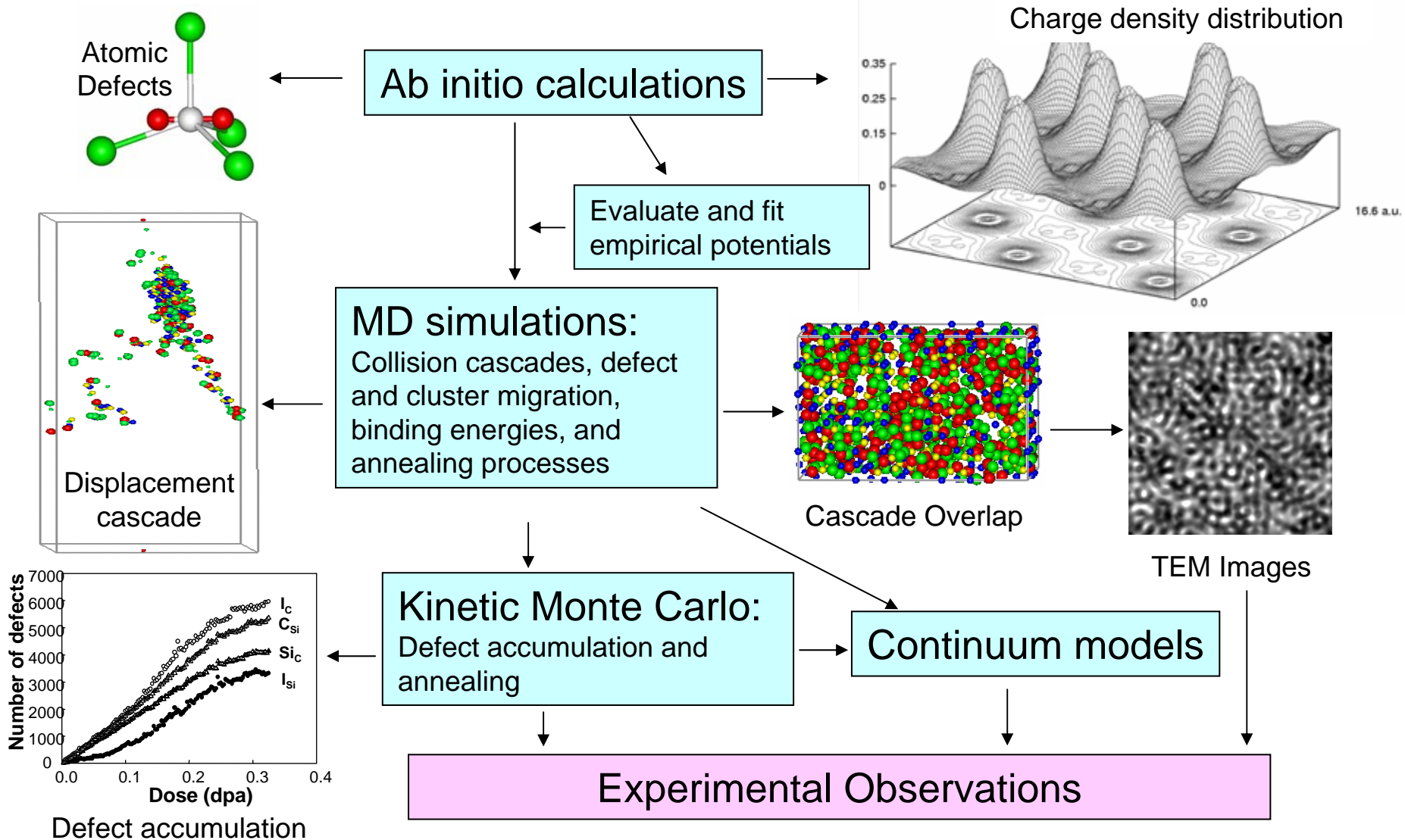atomistic
finite-element
kinetic Monte Carlo
phase field

…

Materials Systems

fuel
structural components
waste forms, …

Needs for high-end computing

Sequential Multi-Scale Modeling in SiC

Atomic Defects

Charge density distribution

Ab initio calculations

Evaluate and fit empirical potentials

MD simulations:
Collision cascades, defect and cluster migration, binding energies, and annealing processes

Displacement cascade

Cascade Overlap

TEM Images

Kinetic Monte Carlo:
Defect accumulation and annealing

Continuum models

Defect accumulation

Experimental Observations

Need is for true multi-scale modeling that passes both directions!
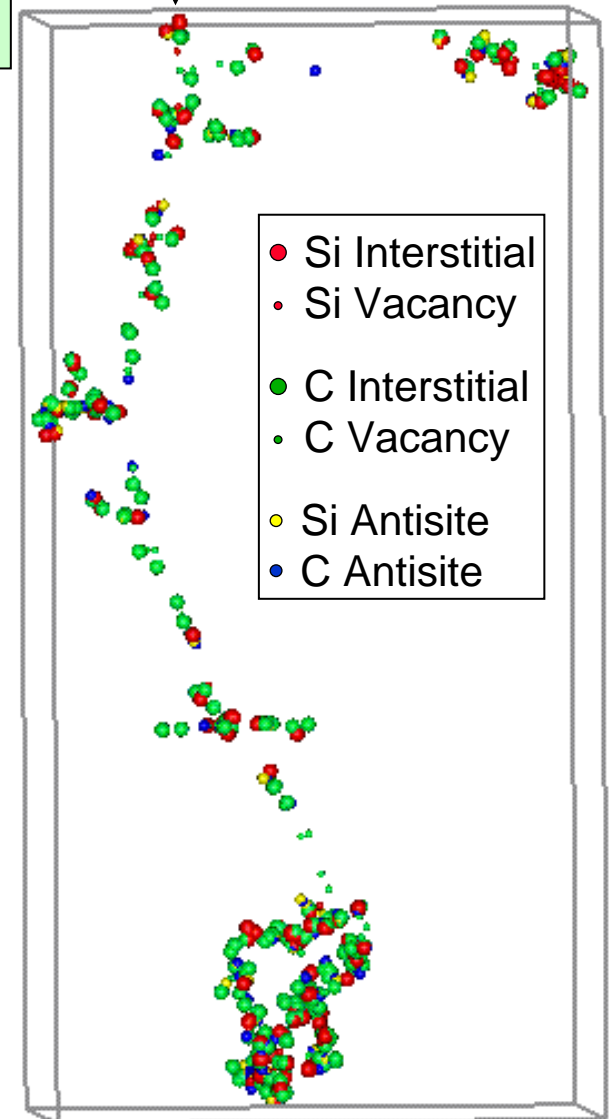
MD Simulation of 50 keV Si Cascade in 3C-SiC

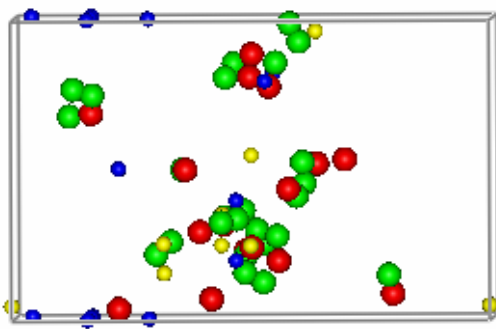Time dependence and spatial distribution of defect production in a 50 keV Si cascade
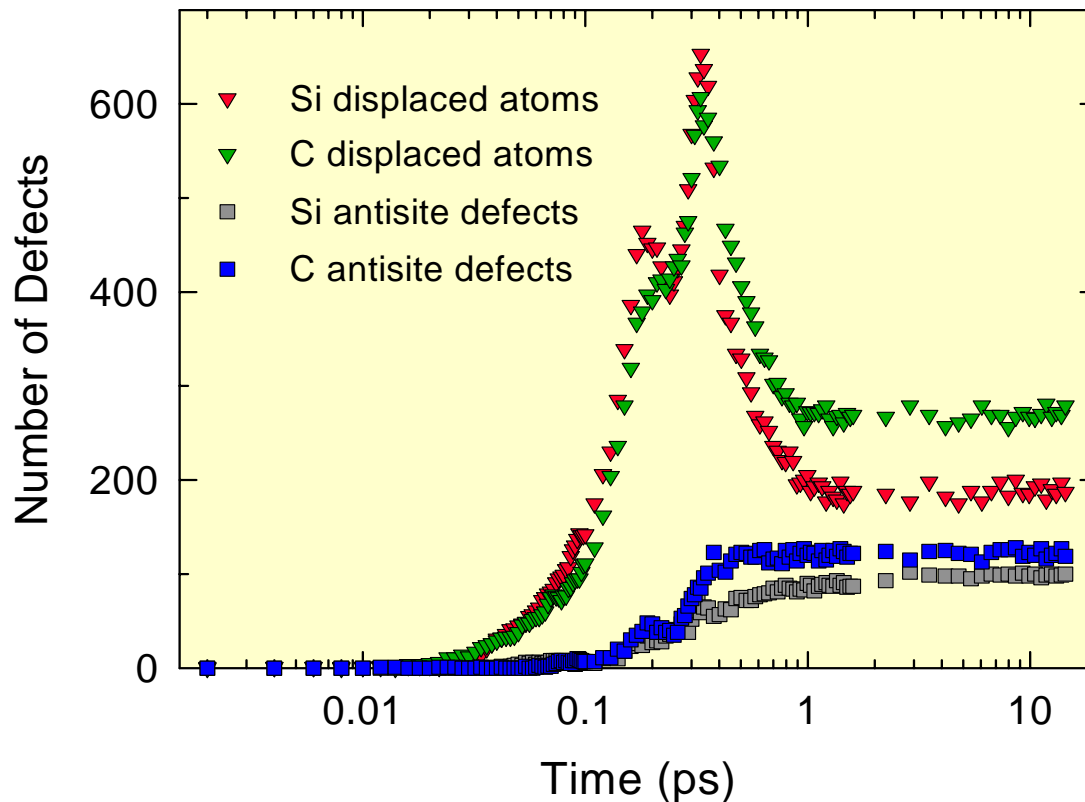
50 keV Si

More C defects than Si defects are produced

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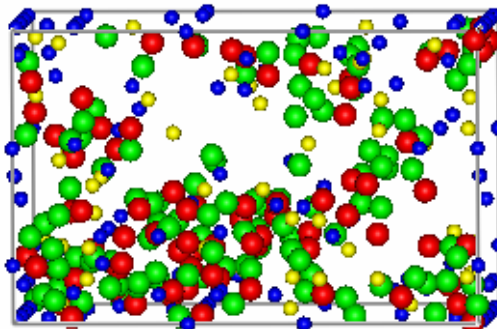
U.S. DEPARTMENT OF ENERGY
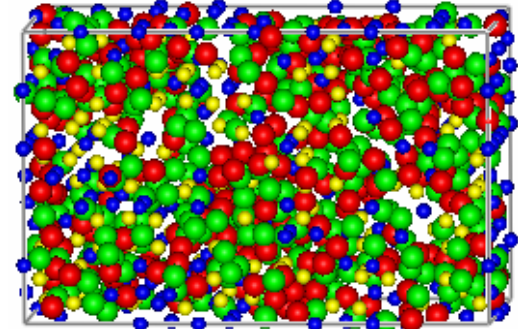
MD Simulations of Cascade Overlap Damage in SiC
Random 10 keV Si Recoils at 200 K (Total of 140 Si Recoils)

0.05 dpa **0.13 dpa** **0.28 dpa**

Disorder from MD Cascades

Relative Disorder vs Dose (dpa)

▲ MD Results
■ Experiment

Simulated Image of MD Damage

2 nm

0.13 dpa

Experimental Image of Ion Damage
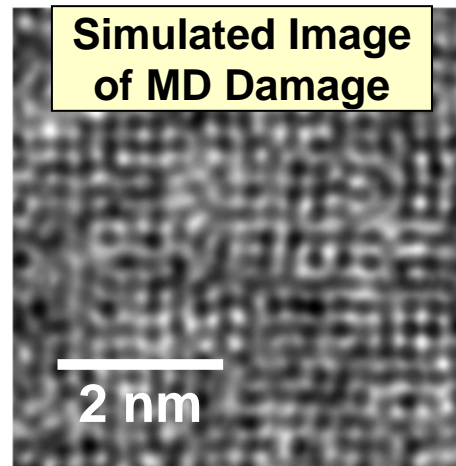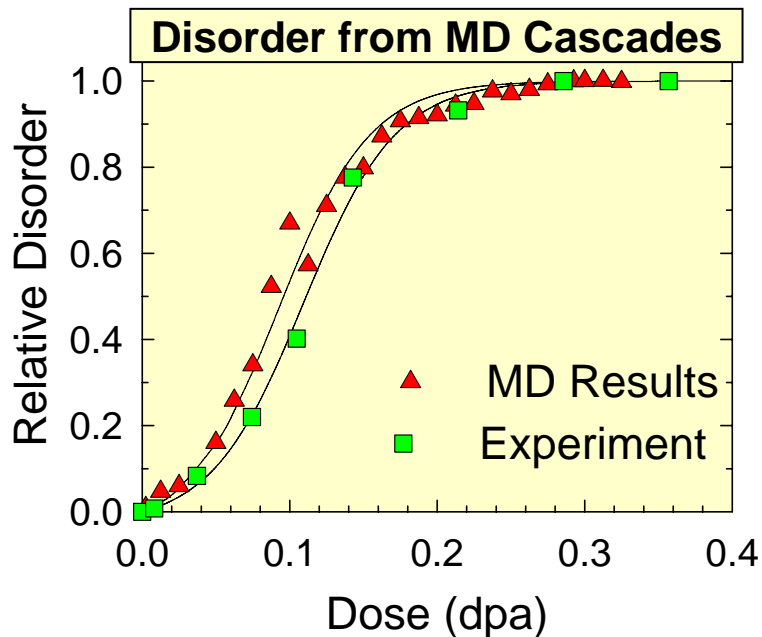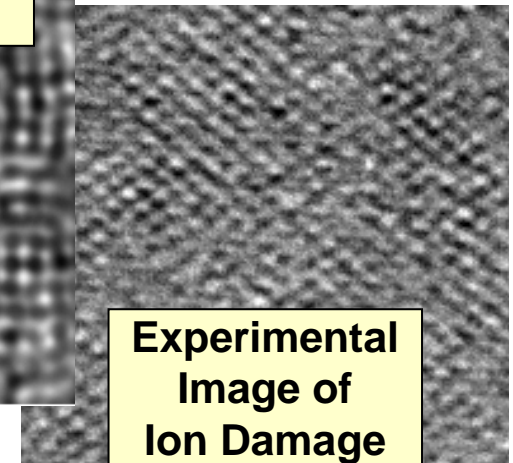
Disorder Accumulation & Simulated Images from MD are in Good Agreement with Experimental Data

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MD Simulation of Self-Interstitial Diffusion

Trajectory of C^+-C<100> Interstitial
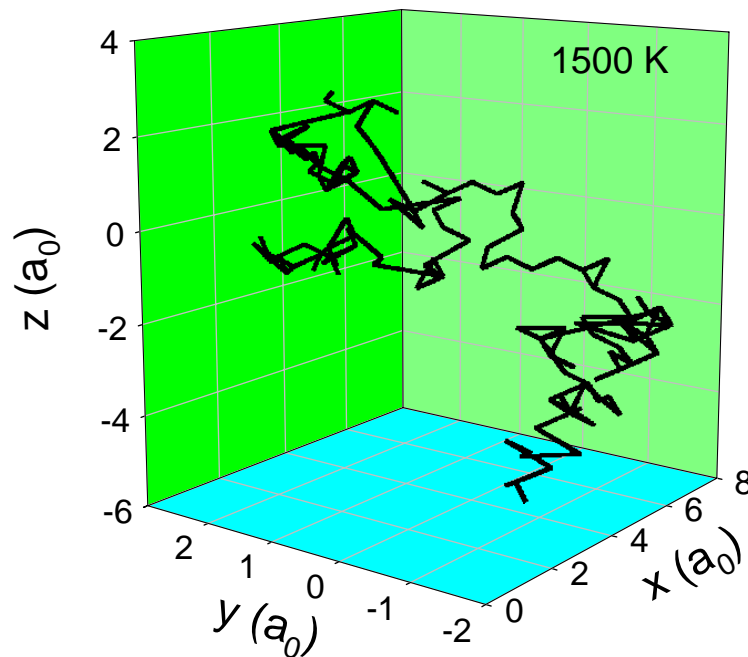
➤ The single interstitial diffuses three-dimensionally

➤ The diffusion mechanism is rather complicated

From Temperature Dependence

➤ Activation energy for C^+-C<100> interstitial ~ 0.74 eV

➤ Activation energy for Si_{TC} interstitial ~ 1.48 eV
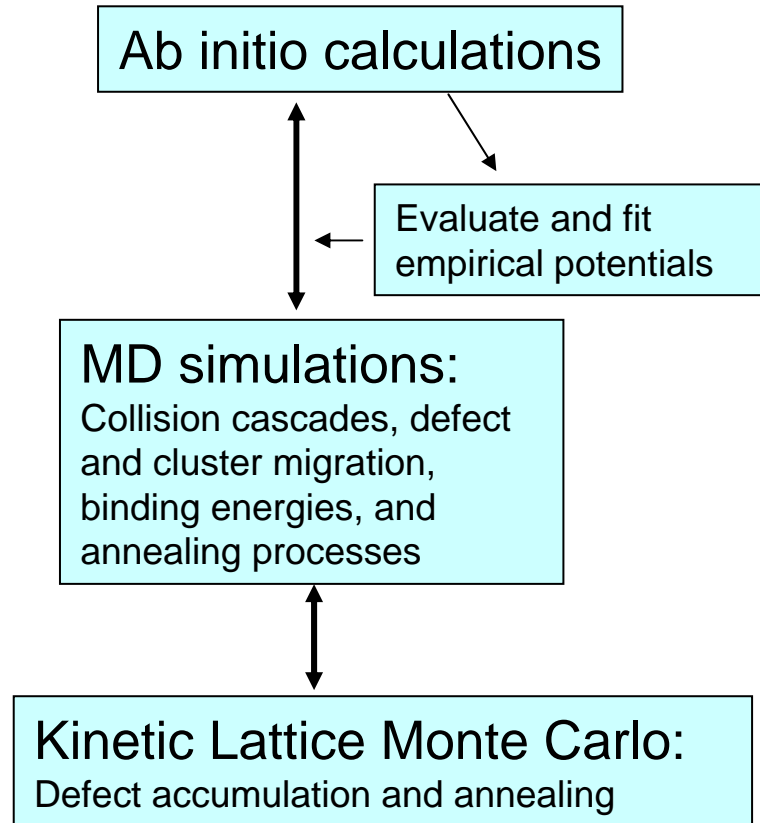
Materials/Radiation Effects Grand Challenges

➢ Predictive models of materials performance under reactor irradiation conditions that are currently unavailable for materials testing

➢ Fission fragment damage, neutron damage, fission gas transport/interactions, and microstructure evolution (e.g., rim-effect) in nuclear fuels

➢ Microstructure evolution, swelling and properties in structural materials (metal alloys, metal carbides, and composites) due to accumulation of radiation-induced defects and helium

➢ Radiation effects in new nuclear waste forms; ionization can cause metastable phase formation, decomposition, and enhanced ion exchange

➢ The effects of electronic excitations on atomic interactions, relaxations, and transport (important for accelerated ion irradiation validation, some in-reactor components and waste forms)

➢ The effects of nanostructures on radiation damage performance

Computational Grand Challenges

➢ Available codes that address materials grand challenges and take advantage of leadership-class computational resources

➢ Development of *ab initio* based methods for generating computationally efficient and robust interatomic potentials

➢ Development of advanced methods that couple atomic dynamics and kinetic Monte Carlo methods

➢ Development of novel multiscale algorithms that link atomistic simulations to phase-field modeling, as well as to continuum deformation and fracture models and corrosion models

➢ New approaches for atomistic simulations in materials with mixed ionic and covalent bonding (includes many oxides, carbides, and nitrides)

➢ Coupling of Atomic and Electronic Dynamics (effects of electronic excitations)

Multi-Scale Modeling of Electronic & Atomic Dynamics

Atomic Dynamics

Ab initio calculations

Evaluate and fit empirical potentials

MD simulations:
Collision cascades, defect and cluster migration, binding energies, and annealing processes

Kinetic Lattice Monte Carlo:
Defect accumulation and annealing

Electronic Dynamics

Ab initio calculations

Parameterize or course-grain the physics

Kinetic Monte Carlo:
Electron-electron interactions and electron-atom interactions

Kinetic Monte Carlo:
Couple electron and atom dynamics